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Direct Determination of Molecular Handedness via Coulomb Explosion Imaging

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Synopsis In this work, we show that the direct determination of a chiral molecule's absolute configuration can be achieved with Coulomb Explosion Imaging in a COLTRIMS reaction microscope. We compare the results after ionisation with femto-second laser pulses and with X-ray synchrotron light. Different fragmentation pathways of the prototypical chiral molecule CHBrClF are identified that carry information on the handedness. The applicabilty of the technique towards bigger molecules is discussed.

Symmetries and asymmetries have always been intriguing phenomena for mankind. In molecular physics and chemistry, the notion of chirality (handedness) plays an important role: Many molecules exist in two forms that are mirror images of each other, like our hands. These two forms of the molecules are commonly called enantiomers. Apart from intellectual curiosity, there is practical interest for the investigation of chiral molecules in pharmacology.

Whereas many techniques exist to distinguish enantiomers, e.g. via optical or vibrational spectroscopy, the determination of the absolute molecular configuration, i.e. the geometry of the underlying structure model, is still challenging. This is especially the case for substances that usually exist in the gas phase.

In the present work, we show that absolute configuration can be determined on a single-molecule level via Coulomb Explosion Imaging (see also [1]). For this purpose, the chiral methane derivative CHBrClF is expanded into a supersonic jet and crossed with laser or synchrotron radiation. After ionisation and fragmentation, the resulting ions are recorded with a COLTRIMS setup [2]. Ionisation by an intense femtosecond laser pulse leads to five-fold ionisation and subsequent fragmentation into atomic ions. From the momenta of these ions, the absolute configuration can be inferred for individual molecules [3]. Figure 1 shows the momenta in the molecular frame of reference. As complete fragmentation is becoming less likely with increasing complexity of the molecules, the possibility of partial fragmentation for the determination of absolute configuration needs to be considered. Results show that fragmentation pathways involving molecular ions can be used to distinguish enantiomers.

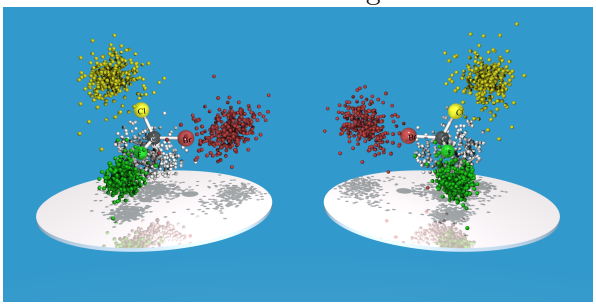

Figure 1. Momenta in the molecular frame for the fragmentation of CHBrClf into Br^+ (red), Cl^+ (yellow), F^+ (green), H^+ (white), C^+ (black arrow) after ionisation with a femtosecond laser pulse.

In a subsequent experiment, it could be demonstrated that also ionisation by a single X-ray photon from a synchrotron source leads to five-fold ionisation and complete fragmentation, as well as to various fragmentation patterns involving neutral fragments. Even though the neutral dissociation products cannot be detected by spectroscopic methods, these break-up channels carry a sign of handedness, increasing the possibility to extend the method towards larger molecules.

References

[1] Ph. Herwig *et al* 2013 *Science* **342** 1084
[2] R. Dörner *et al* 2000 *Physics Reports* **330** 95
[3] M. Pitzer *et al* 2013 *Science* **341** 1096

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